

A rational approximant for the digamma function

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Abstract. Power series representations for special functions are computationally satisfactory only in the vicinity of the expansion point. Thus, it is an obvious idea to use instead Padé approximants or other rational functions constructed from sequence transformations. However, neither Padé approximants nor sequence transformation utilize the information which is available in the case of a special function – all power series coefficients as well as the truncation errors are explicitly known – in an optimal way. Thus, alternative rational approximants, which can profit from additional information of that kind, would be desirable. It is shown that in this way a rational approximant for the digamma function can be constructed which possesses a transformation error given by an explicitly known series expansion.

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Dedicated to Claude Brezinski

1. Introduction

Power series are among the most important tools of calculus. For example, they are extremely useful for the construction of solutions to differential equations. Accordingly, many special functions are defined and computed via power series.

However, from a purely numerical point of view, a power series representation is a mixed blessing. Power series converge well only in the vicinity of the expansion point. Further away, they converge slowly or even diverge. Consequently, the defining power series alone normally does not suffice for an efficient and reliable computation of a special function.

In applied mathematics and in theoretical physics, Padé approximants have become the standard tool to overcome convergence prob-



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lems with slowly convergent or divergent power series [2]. Therefore, it looks like an obvious idea to use them for the computation of special functions.

Padé approximants are defined as solutions of a system of nonlinear equations [2], although they are in practice more often computed by recursive algorithms, for example by Wynn's epsilon algorithm [17]. All these algorithms only need the input of the numerical values of the leading series coefficients. No further information about the function, which is to be approximated, is needed. This is a very advantageous feature, in particular if apart from a finite number of series coefficients very little else is known, and it has undoubtedly contributed significantly to the popularity of Padé approximants and their practical usefulness.

If, however, we want to compute a special function, we are in a much better situation. Not only do we know explicitly *all* coefficients of the power series, but we are also able to write down at least formally explicit expressions for the truncation errors. An approximation scheme for a special function should be able to benefit from additional information of that kind, but Padé approximants – due to their very nature – cannot. Thus, valuable information is wasted, and Padé approximants are in the case of special functions normally less effective than other sequence transformations which can utilize information of that kind. For example, it was shown in [12, 13, 14, 15, 16] that Levin's sequence transformation [5] and some generalizations [12, Sections 7 - 9] can be much more effective than Padé approximants, in particular if factorially divergent asymptotic series for special functions have to be summed.

The power of Levin-type transformations, which were recently reviewed by Homeier [4], is due to the fact that they use as input data not only the elements of the sequence to be transformed but also explicit truncation error estimates. In the majority of all applications, only some very simple truncation error estimates introduced by Levin [5] and Smith and Ford [11] are used. In the case of special functions, however, it may well be possible to derive more sophisticated truncation error estimates which should ultimately lead to more effective approximations. Further research into this direction would be highly desirable.

In the case of special functions, it is also possible to pursue a more direct approach. As discussed for example in [3, 12], a sequence transformation is a map, which transforms a slowly convergent or divergent sequence $\{s_n\}_{n=0}^{\infty}$, whose elements may for instance be the partial sums of an infinite series, into another sequence $\{s'_n\}_{n=0}^{\infty}$ with hopefully better numerical properties. Concerning the input sequence it is assumed that its elements can for all $n \in \mathbb{N}_0$ be partitioned into a (generalized) limit s and a remainder r_n according to $s_n = s + r_n$. A sequence

transformation tries to determine and eliminate the remainders r_n from the sequence elements s_n . Unfortunately, a *complete* elimination of the remainders can normally be accomplished only in the case of more or less artificial model problems. Thus, the elements of the transformed sequence can also be partitioned according to $s'_n = s + r'_n$ into the *same* (generalized) limit s and a transformed remainder r'_n which is normally nonzero for all finite values of n . The transformation process was successful if the transformed remainders $\{r'_n\}_{n=0}^{\infty}$ have better numerical properties than the original remainders $\{r_n\}_{n=0}^{\infty}$.

Normally, only relatively little is known about the remainders r_n . In the case of special functions, however, the situation is much better: *All* coefficients of the power series are explicitly known, and the truncation errors of the partial sums of the power series are at least in principle also explicitly known. Thus, it should be possible to optimize the determination and elimination of the remainders – or equivalently the transformation process – by utilizing the available information as effectively as possible.

It is the intention of this article to show that these goals can be accomplished in the case of the psi or digamma function [1, Eq. (6.3.1)]

$$\psi(z) = \frac{d}{dz} \ln(\Gamma(z)) = \frac{\Gamma'(z)}{\Gamma(z)}, \quad (1.1)$$

which is a meromorphic function with poles at $z = 0, -1, -2, \dots$. Our starting point is the power series representation [1, Eq. (6.3.14)]

$$\psi(1+z) = -\gamma + z\mathcal{Z}(z), \quad (1.2a)$$

$$\mathcal{Z}(z) = \sum_{\nu=0}^{\infty} \zeta(\nu+2)(-z)^{\nu}, \quad (1.2b)$$

which converges for $|z| < 1$. Here, γ is Euler's constant [1, Eq. (6.1.3)] and $\zeta(\nu+2)$ is a Riemann zeta function [1, Eq. (23.2.1)].

2. The transformation of the power series

In this article, an explicit rational approximant for $\mathcal{Z}(z)$ will be constructed. We only have to consider $0 < z < 1$. For $z < 0$, we can use the reflection formula $\psi(1-z) = \psi(z) + \pi \coth(\pi z)$ [1, Eq. (6.3.5)], and for $z \geq 1$, we can use the recurrence formula $\psi(z+1) = \psi(z) + 1/z$ [1, Eq. (6.3.5)]. If the argument z is very large, the digamma function should of course be computed via its asymptotic expansion [1, Eq. (6.3.18)].

For our purposes, it is convenient to rewrite (1.2b) as follows:

$$\mathcal{Z}(z) = \mathcal{Z}_n(z) + \mathcal{R}_n(z), \quad (2.1a)$$

$$\mathcal{Z}_n(z) = \sum_{\nu=0}^n \zeta(\nu+2) (-z)^\nu, \quad (2.1b)$$

$$\mathcal{R}_n(z) = (-z)^{n+1} \sum_{\nu=0}^{\infty} \zeta(n+\nu+3) (-z)^\nu. \quad (2.1c)$$

As discussed in the previous section, a rational approximant to $\mathcal{Z}(z)$ can only improve convergence if the truncation errors $\mathcal{R}_n(z)$ are transformed into other truncation errors with better numerical properties. Thus, we first have to rewrite $\mathcal{R}_n(z)$ in such a way that we better understand its nature. This can be achieved by replacing the zeta functions $\zeta(n+\nu+3)$ in (2.1c) by their Dirichlet series [1, Eq. (23.2.1)] and by interchanging the order of summations. The resulting inner series is a geometric series and can be expressed in closed form. Thus, we obtain

$$\mathcal{Z}_n(z) = \mathcal{Z}(z) - (-1)^{n+1} \sum_{m=0}^{\infty} \frac{[z/(m+1)]^{n+1}}{(m+1)(m+z+1)}. \quad (2.2)$$

This relationship, which holds for all $z \neq -1, -2, -3, \dots$, shows that the partial sums $\mathcal{Z}_n(z)$ are a special case of the following class of sequences with $q_j = z/j$ and $c_j = -1/[j(j+z)]$:

$$s_n = s + (-1)^{n+1} \sum_{j=1}^{\infty} c_j (q_j)^{n+1}, \quad n \in \mathbb{N}_0. \quad (2.3)$$

Concerning the q_j 's, we assume that they all have the same sign and are ordered in magnitude according to

$$1 > |q_1| > |q_2| > \dots > |q_l| > |q_{l+1}| > \dots \geq 0, \quad (2.4)$$

whereas the c_j 's are unspecified coefficients.

Wynn [18] showed that the convergence of a sequence of the type of (2.3) can be accelerated with the help of his epsilon algorithm [17]:

$$\epsilon_{-1}^{(n)} = 0, \quad \epsilon_0^{(n)} = s_n, \quad n \in \mathbb{N}_0, \quad (2.5a)$$

$$\epsilon_{k+1}^{(n)} = \epsilon_{k-1}^{(n+1)} + 1/[\epsilon_k^{(n+1)} - \epsilon_k^{(n)}], \quad k, n \in \mathbb{N}_0. \quad (2.5b)$$

The epsilon algorithm requires as input data only the numerical values of the elements of the sequence (2.3), but not the values of the q_j 's. Wynn also derived asymptotic estimates for the transformation errors $s - \epsilon_{2k}^{(n)}$ [18, Theorems 16 and 17], which were later extended by Sidi [10].

Although the epsilon algorithm is a very powerful accelerator for sequences of type of (2.3) – numerical studies showed that the epsilon

algorithm accelerates the convergence of the power series in (1.2b) much more effectively than for example Levin's transformation [5] or some generalizations [12, Sections 7 - 9] – it nevertheless cannot profit from the fact that in the case of (2.2) the q_j are explicitly known. Moreover, no explicit expressions for the rational approximants or the transformation errors are known. Thus, we use instead the sequence transformation

$$T_k^{(n)} = T_k^{(n)}(s_n, \dots, s_{n+k}) = \prod_{\kappa=1}^k \frac{E + q_\kappa}{1 + q_\kappa} s_n \quad (2.6)$$

as the starting point for the construction of an explicit rational approximant to $\mathcal{Z}(z)$. Here, E is the shift operator defined by $Ef(n) = f(n+1)$.

The sequence transformation $T_k^{(n)}$ can also be computed recursively:

$$T_0^{(n)} = s_n, \quad n \in \mathbb{N}_0, \quad (2.7a)$$

$$T_{k+1}^{(n)} = \frac{T_k^{(n+1)} + q_{k+1} T_k^{(n)}}{1 + q_{k+1}}, \quad k, n \in \mathbb{N}_0. \quad (2.7b)$$

Essentially identical sequence transformations were discussed by Matos [8, 9].

An explicit expression for $T_k^{(n)}$ can be derived with the help of the *elementary symmetric polynomials* $e_\nu^{(n)}$ in n variables x_1, \dots, x_n , which are defined by the generating function [6, p. 13]

$$\prod_{j=1}^n (1 + x_j t) = \sum_{\nu=0}^n e_\nu^{(n)} t^\nu. \quad (2.8)$$

The substitution $s = 1/t$ yields the equivalent generating function

$$\prod_{j=1}^n (s + x_j) = \sum_{\nu=0}^n e_{n-\nu}^{(n)} s^\nu. \quad (2.9)$$

Comparison with (2.6) shows that $T_k^{(n)}$ possesses an explicit expression involving the elementary symmetric polynomials $e_\kappa^{(k)}$ in the k variables q_κ with $1 \leq \kappa \leq k$:

$$T_k^{(n)} = \frac{\sum_{\kappa=0}^k e_{k-\kappa}^{(k)}(q_1, \dots, q_k) E^\kappa s_n}{\sum_{\kappa=0}^k e_\kappa^{(k)}(q_1, \dots, q_k)} = \frac{\sum_{\kappa=0}^k e_{k-\kappa}^{(k)}(q_1, \dots, q_k) s_{n+\kappa}}{\sum_{\kappa=0}^k e_\kappa^{(k)}(q_1, \dots, q_k)}. \quad (2.10)$$

In most practical applications, the sequence transformation $T_k^{(n)}$ is not particularly useful since the values of the q_j 's have to be explicitly known. If, however, this is the case and if the input data are the elements of the sequence (2.3), then it can be shown by complete induction in k that

$$T_k^{(n)} = s + (-1)^{n+1} \sum_{j=k+1}^{\infty} c_j \prod_{\kappa=1}^k \frac{q_{\kappa} - q_j}{q_{\kappa} + 1} (q_j)^{n+1}. \quad (2.11)$$

Thus, the first k exponential terms $c_j(q_j)^{n+1}$ in (2.3) are eliminated. Since the q_j 's are by assumption ordered in magnitude according to (2.4), this leads to an acceleration of convergence. Moreover, the application of $T_k^{(n)}$ to the elements of the sequence (2.3) leads for sufficiently large values of k to a convergent sequence if the original sequence diverges because the leading q_j 's in (2.3) satisfy $|q_j| > 1$.

Combination of (2.2) and (2.11) yields the following explicit rational approximant to $\mathcal{Z}(z)$:

$$\begin{aligned} T_n^{(k)}(\mathcal{Z}_n(z), \dots, \mathcal{Z}_{n+k}(z)) &= \prod_{\kappa=1}^k \frac{E + (z/\kappa)}{1 + (z/\kappa)} \mathcal{Z}_n(z) = \mathcal{Z}(z) \\ &- (-1)^{n+1} \frac{z^{n+k+1}}{(z+1)_k} \sum_{m=0}^{\infty} \frac{(m+1)_k}{(k+m+1)^{n+k+2}(k+m+z+1)} \end{aligned} \quad (2.12)$$

Here, $(z+1)_k$ and $(m+1)_k$ are Pochhammer symbols. It is a remarkable feature of this rational approximant that its transformation error possesses an explicit series expansion. This is quite uncommon in the theory of rational approximants. Moreover, the first k poles of $\mathcal{Z}(z)$ at $z = -1, -2, \dots, -k$ are reproduced by $T_k^{(n)}$, whereas the remaining poles at $z = -k-1, -k-2, \dots$ are reproduced by the infinite series for the transformation error.

The prefactor of the infinite series in (2.12) can be expressed as a beta function $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$ [1, Eq. (6.2.2)] according to

$$\frac{z^{n+k+1}}{(z+1)_k} = \frac{z^{n+k+2}}{k!} B(z, k+1). \quad (2.13)$$

It is possible to derive an alternative expression for the infinite series in (2.12) which more closely resembles the infinite series in (2.2), from which it was derived. For that purpose, we write the Pochhammer symbol in the infinite series in (2.12) as a product according to $(m+1)_k = \prod_{\kappa=1}^k ([k+m+1] + [\kappa - k - 1])$. Comparison with (2.9) shows that this is the generating function of the elementary symmetric polynomials

$\hat{e}_\kappa^{(k)}$ in the k variables $x_\kappa = \kappa - k - 1$ with $1 \leq \kappa \leq k$. Thus, we obtain

$$(m+1)_k = \sum_{\kappa=0}^k \hat{e}_{k-\kappa}^{(k)} (k+m+1)^\kappa = \sum_{\kappa=0}^k \hat{e}_\kappa^{(k)} (k+m+1)^{k-\kappa}. \quad (2.14)$$

Inserting this into (2.12) yields:

$$\begin{aligned} T_n^{(k)}(\mathcal{Z}_n(z), \dots, \mathcal{Z}_{n+k}(z)) &= \mathcal{Z}(z) - (-1)^{n+1} \frac{z^{n+k+1}}{(z+1)_k} \\ &\times \sum_{\kappa=0}^k \hat{e}_\kappa^{(k)} \sum_{m=0}^{\infty} \frac{1}{(k+m+1)^{n+\kappa+2} (k+m+z+1)}. \end{aligned} \quad (2.15)$$

If we now do a Taylor expansion of $1/(k+m+z+1)$ and introduce the generalized (Hurwitz) zeta function $\zeta(z, \alpha) = \sum_{n=0}^{\infty} (n+\alpha)^{-z}$ with $\alpha \neq 0, -1, -2, \dots$ [7, p. 22], we obtain

$$\begin{aligned} &\sum_{m=0}^{\infty} \frac{1}{(k+m+1)^{n+\kappa+2} (k+m+z+1)} \\ &= \sum_{m=0}^{\infty} \zeta(n+m+\kappa+3, k+1) (-z)^m \end{aligned} \quad (2.16)$$

and

$$\begin{aligned} T_n^{(k)}(\mathcal{Z}_n(z), \dots, \mathcal{Z}_{n+k}(z)) &= \mathcal{Z}(z) - (-1)^{n+1} \frac{z^{n+k+1}}{(z+1)_k} \\ &\times \sum_{m=0}^{\infty} (-z)^m \sum_{\kappa=0}^k \hat{e}_\kappa^{(k)} \zeta(n+m+\kappa+3, k+1). \end{aligned} \quad (2.17)$$

Further modifications of (2.17) are possible. For example, ordinary zeta functions can be introduced instead of the generalized (Hurwitz) zeta functions according to

$$\zeta(n+m+\kappa+3, k+1) = \zeta(n+m+\kappa+3) - \sum_{\nu=0}^k (\nu+1)^{-n-m-\kappa-3}. \quad (2.18)$$

For larger values of k , the inner sum in (2.17) is likely to become numerically unstable since the k variables $x_\kappa = \kappa - k - 1$ of the elementary symmetric polynomials $\hat{e}_\kappa^{(k)}$ are all negative. This implies that the $\hat{e}_\kappa^{(k)}$ alternate in sign with increasing κ . Thus, sums of the type $\sum_{\kappa=0}^k \hat{e}_\kappa^{(k)} f_\kappa$ seem to have similar properties as sums of the type $\sum_{\kappa=0}^k (-1)^\kappa \binom{k}{\kappa} f_\kappa$ which are known to be numerical unstable for larger values of k if all f_κ have the same sign.

3. Numerical examples

We now want to show that the new explicit rational approximant to $\mathcal{Z}(z)$ is indeed a numerically useful tool. Thus, we apply both $T_k^{(n)}$ defined by (2.6) as well as Wynn's epsilon algorithm (2.5) to the partial sums $\mathcal{Z}_n(z)$ defined by (2.1b).

The transforms $T_n^{(k)}$ were computed with the help of the recurrence formula (2.7) which should be the most effective approach. For the recursive calculation, two one-dimensional arrays \mathbf{t} and \mathbf{q} suffice (compare [12, Sections 4.3 and 7.5]):

$$\mathbf{t}[0] \leftarrow s_0, \quad (3.1a)$$

$$\mathbf{t}[m] \leftarrow s_m, \quad \mathbf{q}[m] \leftarrow q_m, \quad m \geq 1, \quad (3.1b)$$

$$\mathbf{t}[m-j] \leftarrow \frac{\mathbf{t}[m-j+1] + \mathbf{q}[j]\mathbf{t}[m-j]}{1 + \mathbf{q}[j]}, \quad 1 \leq j \leq m. \quad (3.1c)$$

For each $m \geq 0$, $\mathbf{t}[0] = T_m^{(0)}$ is used to approximate the limit of the input sequence.

The argument $z = 1$ considered in Table 3 lies on the boundary of the circle of convergence of the power series (1.2b) for $\mathcal{Z}(z)$. The approximants in the last column of Table 3 were chosen according to [12, Eq. 4.3-6].

All calculations in Table 3 were done in MapleV Release 5.1 with an accuracy of 32 decimal digits. When the accuracy was reduced to 16 digits, at most the last digit printed differed. Thus, the computation of the rational approximants in Table 3 is apparently numerically remarkably stable.

The results in Table 3 show that the new rational approximant and Wynn's epsilon algorithm produce results of virtually identical quality. This is also observed in the case of complex arguments. In Table 3, we consider $z = [1 + \sqrt{3}i]/2$ which again lies on the boundary of the circle of convergence of the power series (1.2b) for $\mathcal{Z}(z)$.

In the case of the epsilon algorithm, we obtain in the case of $z = [1 + \sqrt{3}i]/2$:

$$-\gamma + z\epsilon_{14}^{(0)} = 0.285\,073\,441\,270\,305 + 0.691\,215\,820\,928\,757\,\mathfrak{i} \quad (3.2)$$

$$-\gamma + z\epsilon_{14}^{(1)} = 0.285\,073\,441\,270\,304 + 0.691\,215\,820\,928\,755\,\mathfrak{i} \quad (3.3)$$

All calculations in Table 3 were again done with an accuracy of 32 decimal digits. When we reduced the accuracy to 16 digits, we observed as in Table 3 that at most the last digit printed differed.

Wynn's epsilon algorithm is – as already remarked – a very powerful accelerator for sequences of the type of (2.3). Thus, the numerical

Table I. Convergence of the new rational approximant for $\psi(1+z)$ with $z=1$.

n	$-\gamma + z\mathcal{Z}_n(z)$	$-\gamma + zT_n^{(0)}$	$-\gamma + z\epsilon_{2\llbracket n/2 \rrbracket}^{(n-2\llbracket n/2 \rrbracket)}$
0	1.067 718	1.067 718 401 946 694	1.067 718 401 946 694
1	-0.134 339	0.466 689 950 366 896	-0.134 338 501 212 901
2	0.947 985	0.426 778 727 217 411	0.435 187 600 653 266
3	-0.088 943	0.423 160 888 178 296	0.418 415 084 082 869
4	0.928 400	0.422 818 740 326 191	0.422 960 666 980 241
5	-0.079 949	0.422 787 312 867 790	0.422 747 356 295 448
6	0.924 128	0.422 784 577 276 038	0.422 786 030 269 854
7	-0.077 880	0.422 784 353 568 296	0.422 784 084 294 859
8	0.923 114	0.422 784 336 420 153	0.422 784 346 626 811
9	-0.077 380	0.422 784 335 187 365	0.422 784 333 783 337
10	0.922 866	0.422 784 335 104 100	0.422 784 335 156 547
11	-0.077 256	0.422 784 335 098 804	0.422 784 335 093 078
12	0.922 805	0.422 784 335 098 486	0.422 784 335 098 692
13	-0.077 226	0.422 784 335 098 468	0.422 784 335 098 450
14	0.922 789	0.422 784 335 098 467	0.422 784 335 098 467
$\psi(1+z)$		0.422 784 335 098 467	0.422 784 335 098 467

results presented in Tables 3 and 3 indicate that the new rational approximant $T_k^{(n)}$ to $\mathcal{Z}(z)$ is indeed numerically useful for the computation of the digamma function. Nevertheless, further improvements should be possible. For example, we so far completely ignored that we have an explicit series expansion for the transformation error according to (2.12). The convergence of this series can also be accelerated, for instance by Levin's u transformation [5], but unfortunately, its convergence cannot be accelerated as effectively as the convergence of the series (1.2b) for $\mathcal{Z}(z)$. So, most desirable would be an asymptotic expansion for the transformation error in (2.12) as k becomes large. However, this is beyond the scope of the present article.

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Table II. Convergence of the new rational approximant for $\psi(1+z)$ with $z = [1 + \sqrt{3}i]/2$.

n	$-\gamma + z\mathcal{Z}_n(z)$	$-\gamma + zT_n^{(0)}$
0	0.245 + 1.425 i	0.245 251 368 522 580 + 1.424 554 689 441 014 i
1	0.846 + 0.384 i	0.245 251 368 522 580 + 0.730 546 812 820 574 i
2	-0.236 + 0.384 i	0.279 460 988 364 996 + 0.691 044 946 370 787 i
3	0.282 + 1.282 i	0.284 708 842 795 361 + 0.690 769 505 446 420 i
4	0.791 + 0.401 i	0.285 084 829 446 025 + 0.691 160 242 235 571 i
5	-0.217 + 0.401 i	0.285 078 145 123 076 + 0.691 213 499 135 601 i
6	0.285 + 1.270 i	0.285 073 844 960 382 + 0.691 216 025 583 709 i
7	0.786 + 0.402 i	0.285 073 447 077 753 + 0.691 215 856 873 046 i
8	-0.215 + 0.402 i	0.285 073 439 323 115 + 0.691 215 822 849 613 i
9	0.285 + 1.269 i	0.285 073 441 081 160 + 0.691 215 820 893 795 i
10	0.785 + 0.403 i	0.285 073 441 265 135 + 0.691 215 820 917 156 i
11	-0.215 + 0.403 i	0.285 073 441 270 720 + 0.691 215 820 928 085 i
12	0.285 + 1.269 i	0.285 073 441 270 350 + 0.691 215 820 928 754 i
13	0.785 + 0.403 i	0.285 073 441 270 305 + 0.691 215 820 928 757 i
14	-0.215 + 0.403 i	0.285 073 441 270 303 + 0.691 215 820 928 756 i
15	0.285 + 1.269 i	0.285 073 441 270 304 + 0.691 215 820 928 755 i
$\psi(1+z)$		0.285 073 441 270 304 + 0.691 215 820 928 756 i

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